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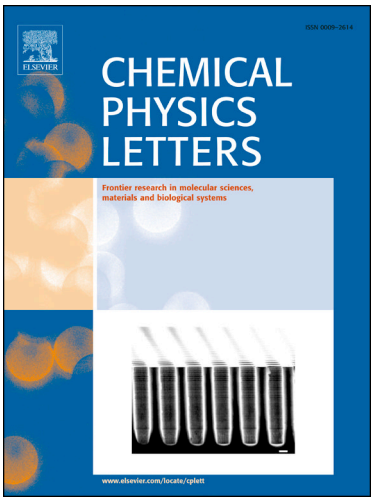

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Katsuhiko Nishiyama

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Exploration of peptides that fit into the thermally vibrating active site of cathepsin K protease by alternating artificial intelligence and molecular simulation

Katsuhiko Nishiyama*

National Institute of Technology, Tsuruoka College, 104 Sawada, Inooka, Tsuruoka, Yamagata 997-8511, Japan

Abstract

Eighteen tripeptides that fit into the thermally vibrating active site of cathepsin K were discovered by alternating artificial intelligence and molecular simulation. The 18 tripeptides fit the active site better than the cysteine protease inhibitor E64, and a better inhibitor of cathepsin K could be designed considering these tripeptides. Among the 18 tripeptides, Phe–Arg–Asp and Tyr–Arg–Asp fit the active site the best and their structural similarity should be considered in the design process. Interesting factors emerged from the structure of the decision tree, and its structural information will guide exploration of potential inhibitor molecules for proteases.

Keywords: Protein, Artificial Intelligence, Molecular Dynamics Simulations, Docking Simulations

1. Introduction

Proteases are targets for the treatment of many diseases[1, 2, 3]. In many cases, their inhibitors are designed based on the structures of peptides that fit into their active sites. Proteases are also used in a wide variety of fields, such as food processing and medical practice [4], and clarification of their substrates would increase the scope of their applications. Discovery of fitted

*phone number +81-235-25-9076
Email address: nisiyama@asagi.waseda.jp (Katsuhiko Nishiyama)

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